Intricacies of Counterflow Flames in Validating Chemical Kinetic Models

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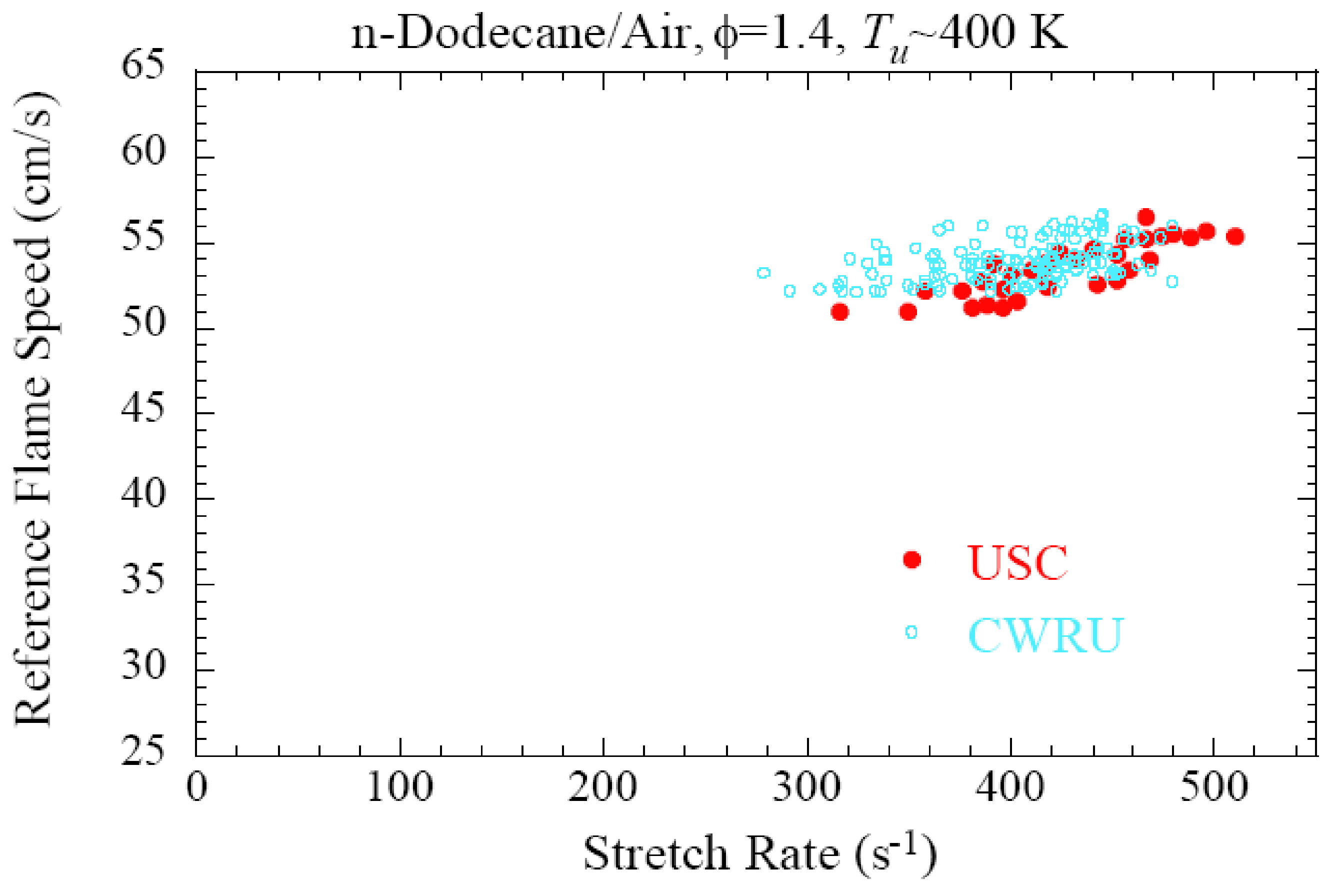
NASA Hypersonics NRA Program

OSD TE & ST Program

Motivation

- Experimental data presented at the last MACCCR Meeting by Jackie Sung



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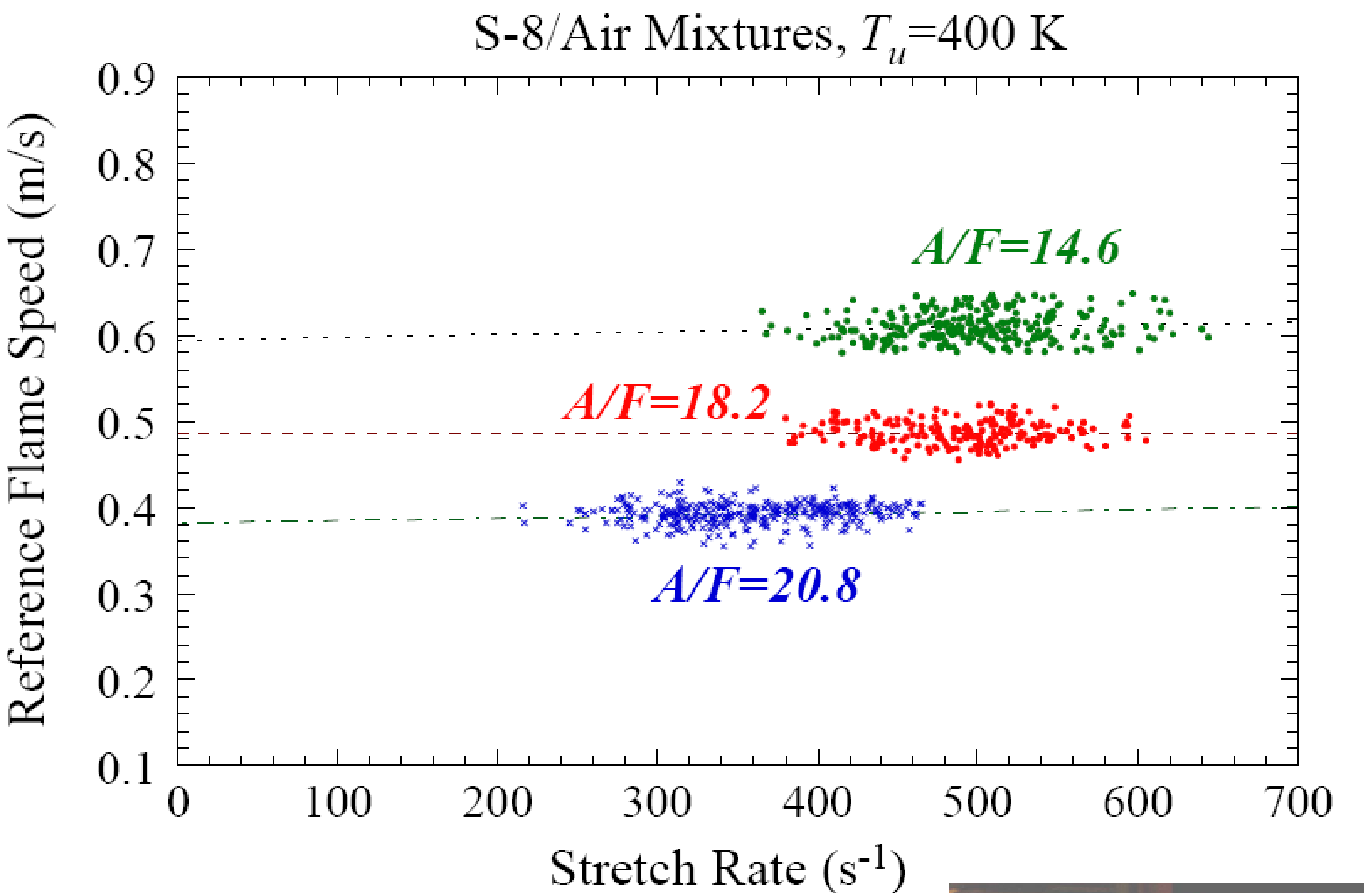

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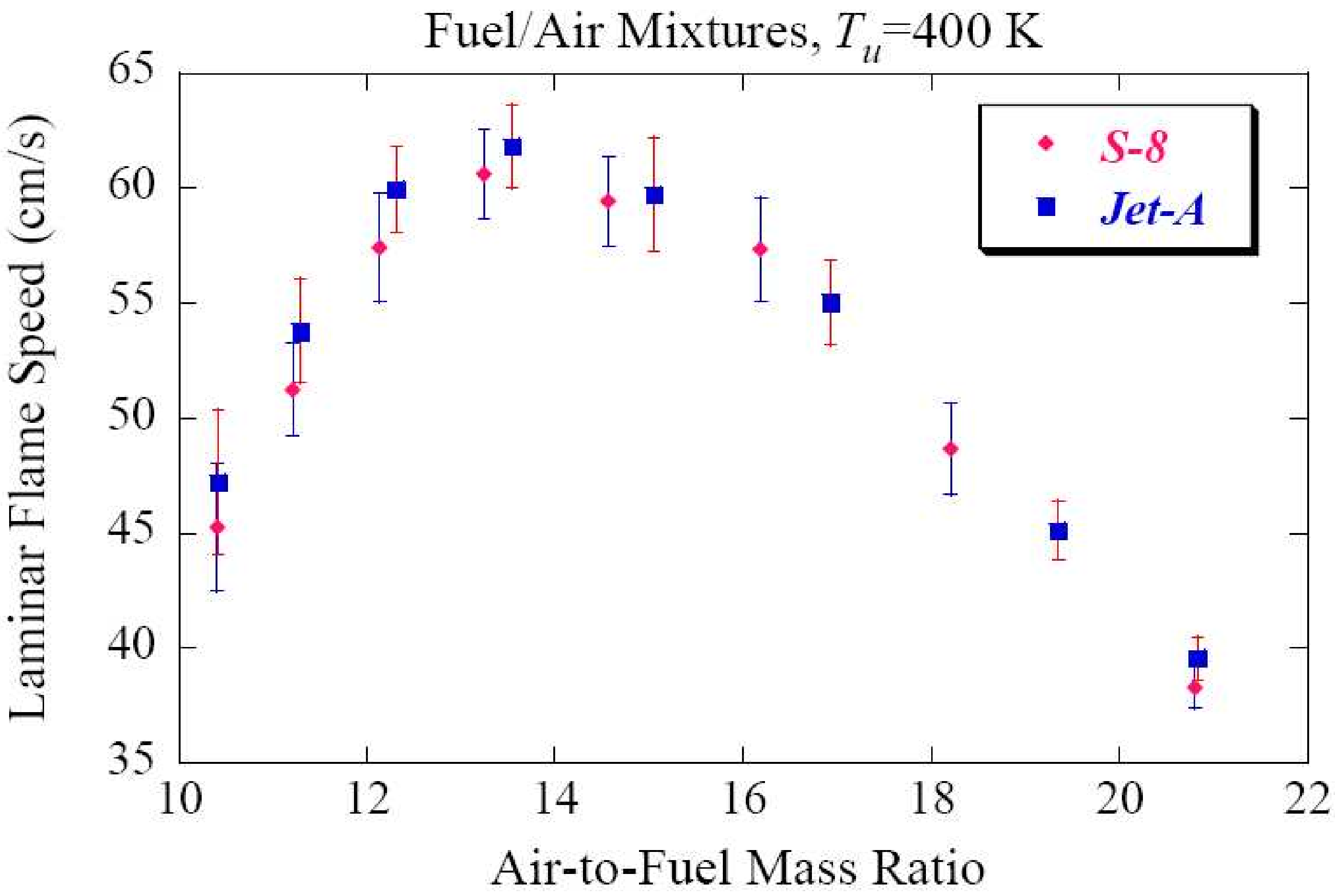

Questions?

- How accurate is the local strain rate, reference velocity, ...?

- Can we use an alternate counterflow flame property for optimization and validation of chemical kinetic models?

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$$\boxed{\text{Extinction Strain Rate of Nonpremixed Flames}}$$

Outline

- A brief review

- Uncertainties of experimental data:
  — premixed flames (last MACCCR Fuels Meeting at NIST)
  — non-premixed flames (eg. ethylene-air data of USC, NASA Langley, and UVa)

- Two-dimensional effects?
  — LDV and PIV data
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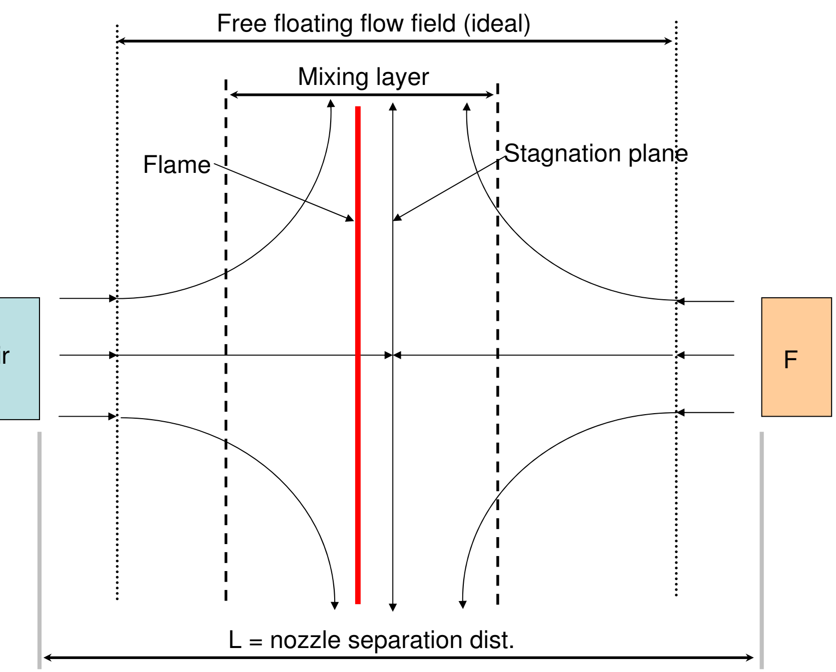
- Mechanism reduction based on principal component/QSSA analyses

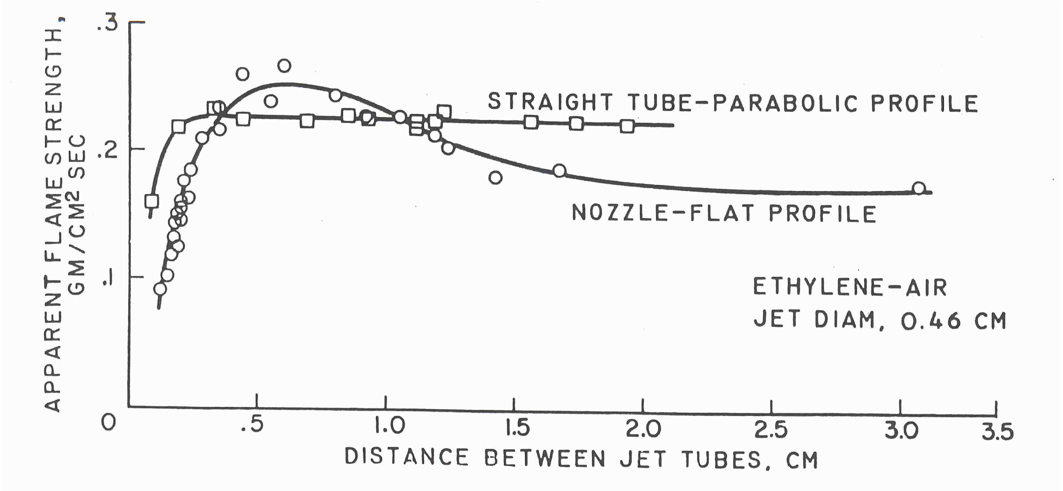
- Concluding remarks

Review - Free-floating Limit

- Ideal, free-floating counterflow field for $L/D > 2$



Ideal case



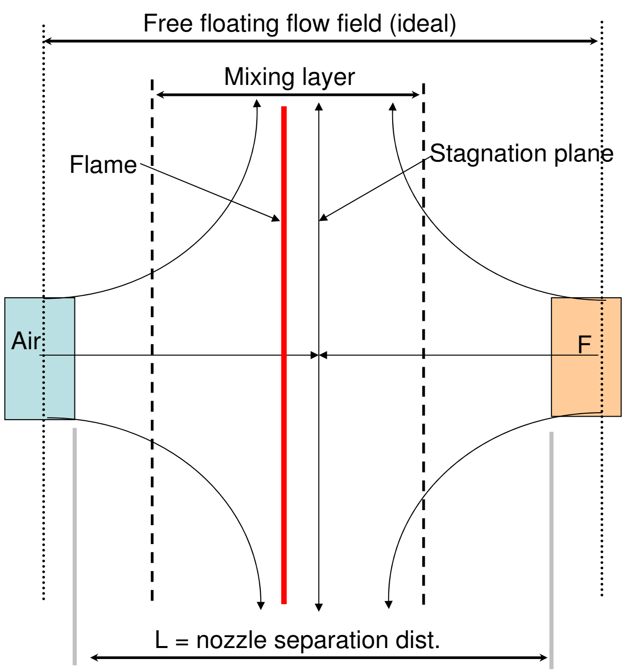
Potter, Heimel, and Buttler

Eighth Combustion Symposium, 1960

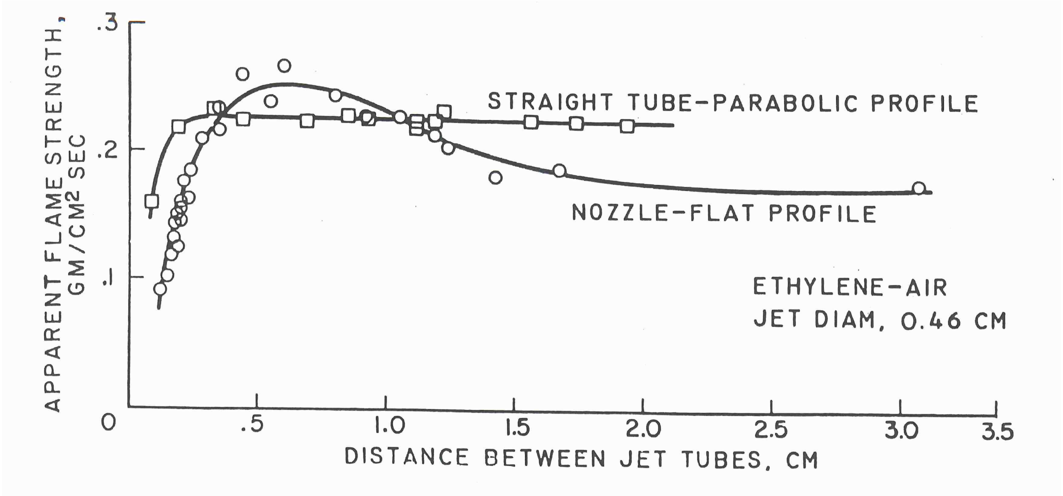
$\boxed{a_{global} \sim 1900s^{-1} \text{ at } L/D \sim 1}$

Review - Free-floating Limit

- Non-ideal counterflow field for $L/D < 1$



Non-ideal case



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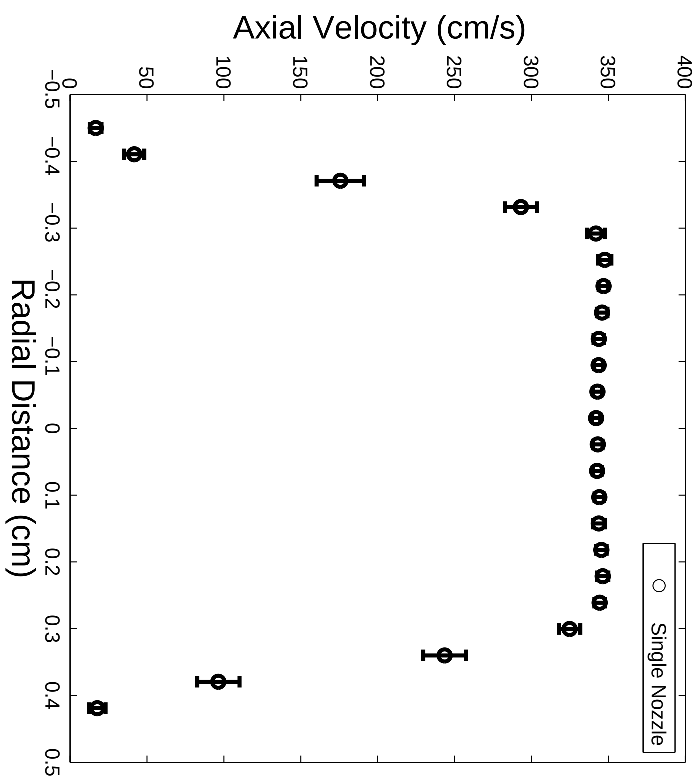
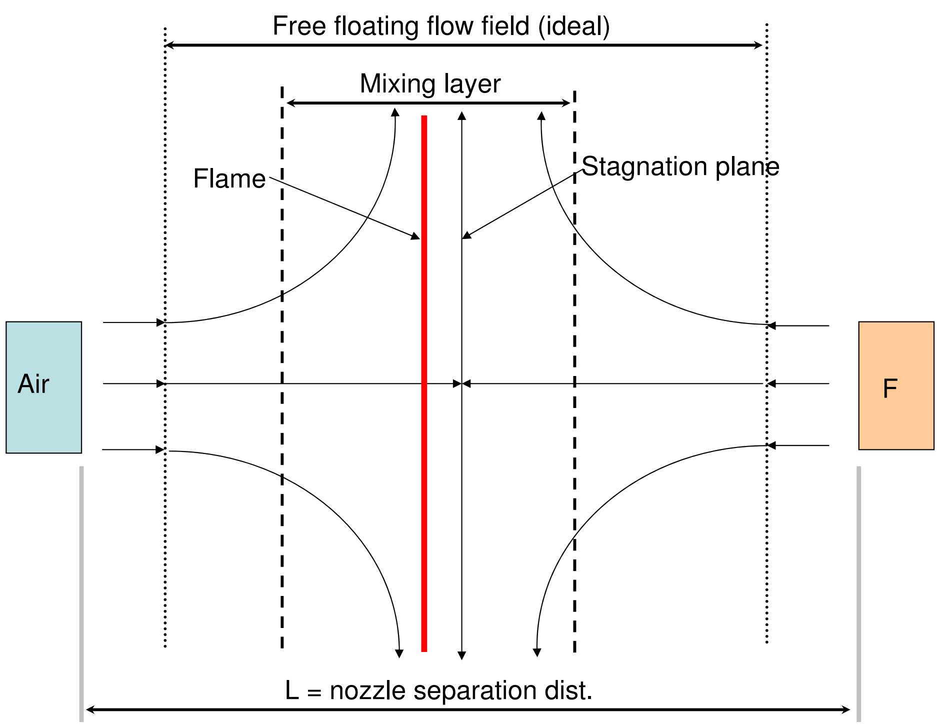
$$\boxed{a_{global} \sim 1900 s^{-1} \text{ at } L/D \sim 1}$$

Review - Influence of Nozzle Exit Profile

- Non-ideal separation distance effect on nozzle exit velocity profile
- First demonstrated by Rolon et al. in early 1990's.





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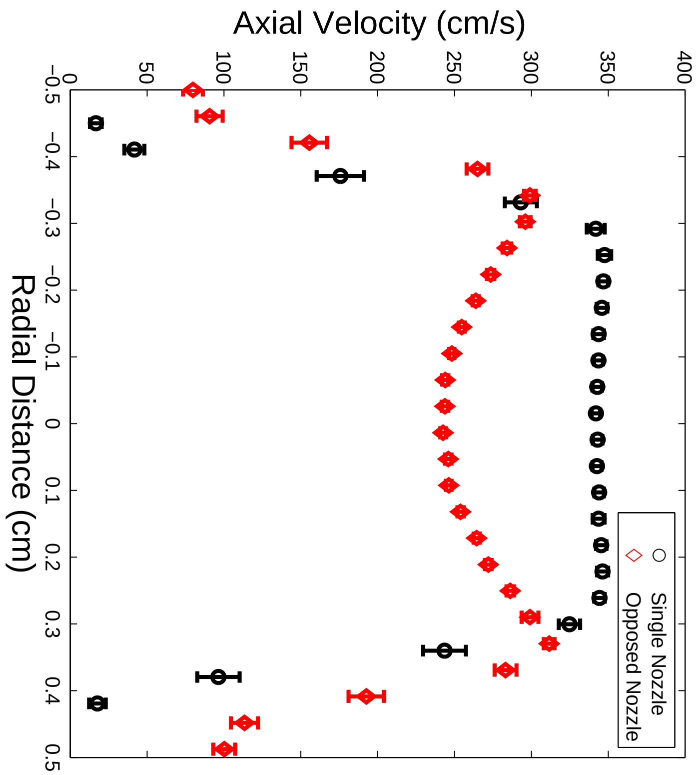
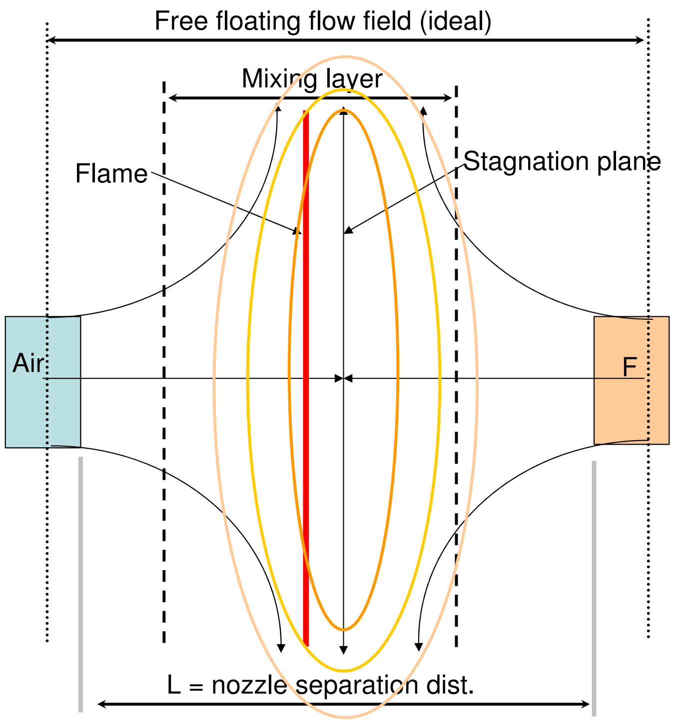
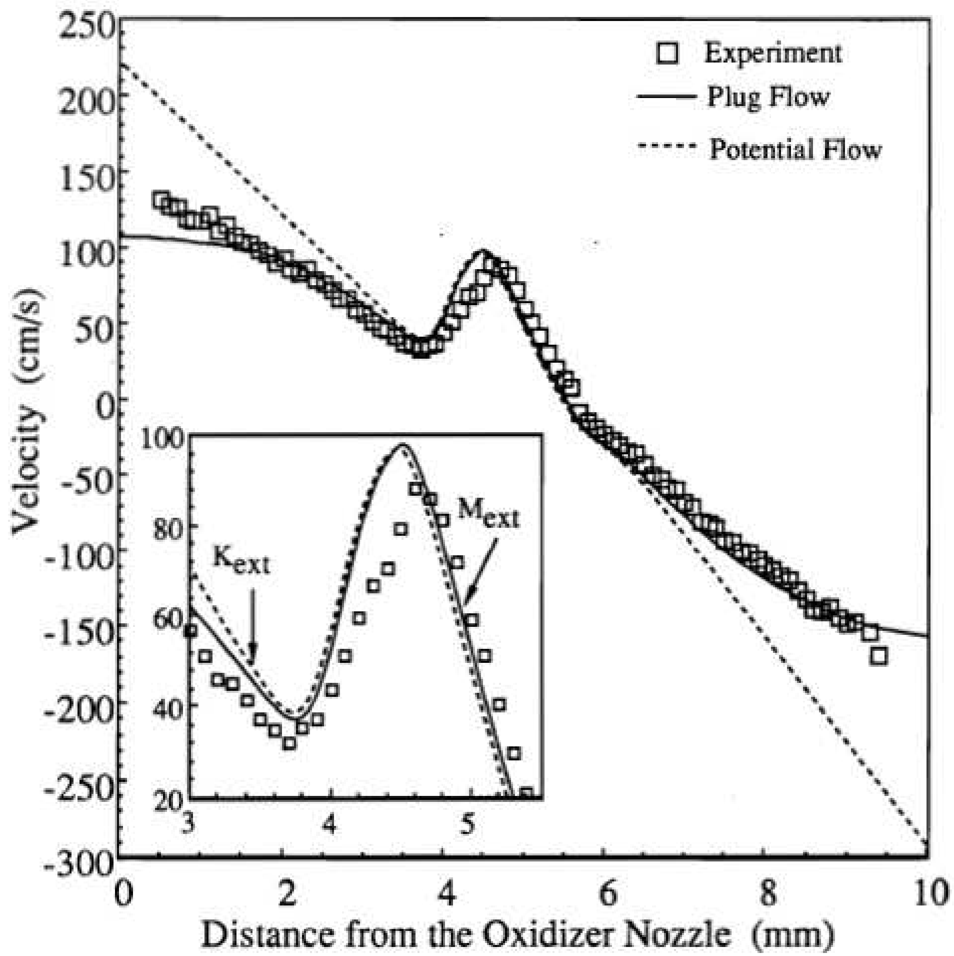




Review - Influence of Radial Boundary Condition

- Finite $\partial v_r/\partial r$ ($\equiv U$) (Chelliah et al., 23rd Symp., 1990, Smooke et al. 1990)
- Axial velocity of methane-air non-premixed flames near extinction



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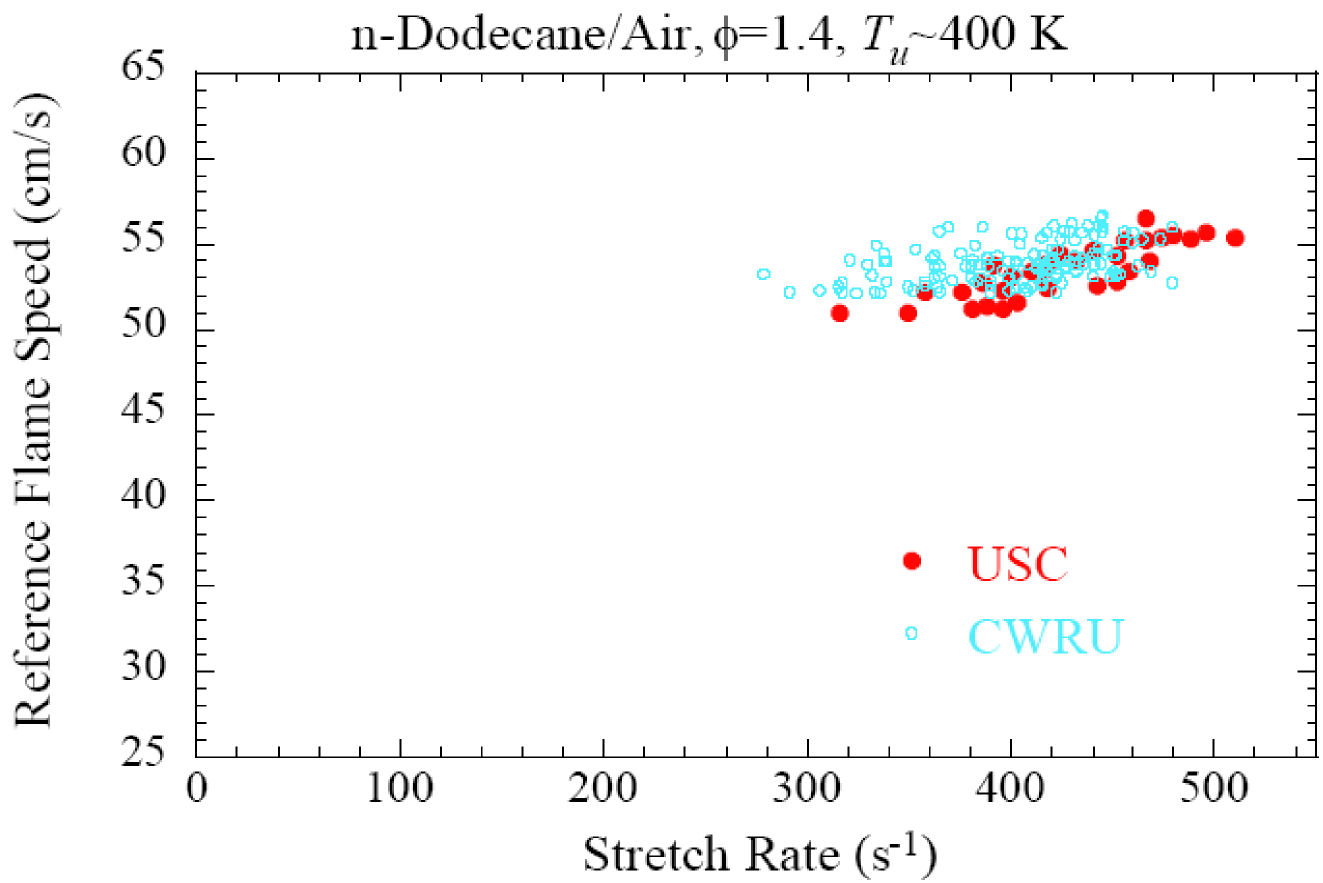
Uncertainties – Burning Velocity of Premixed Flames

- Three key uncertainties

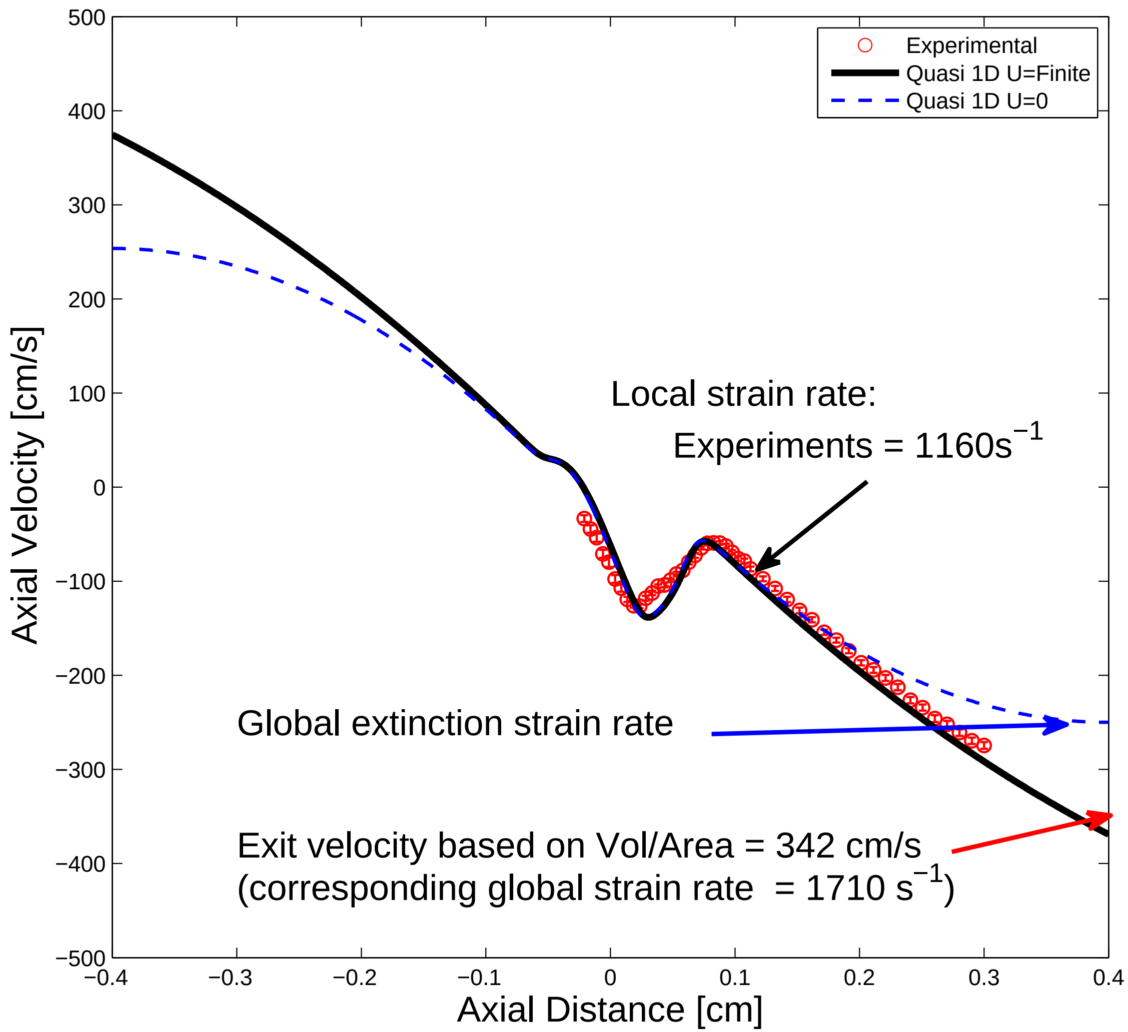
  (i) local strain rate, (ii) reference velocity

  (ii) linear vs. non-linear extrapolation (Stahl, Warnatz, and Rogg, 1988).



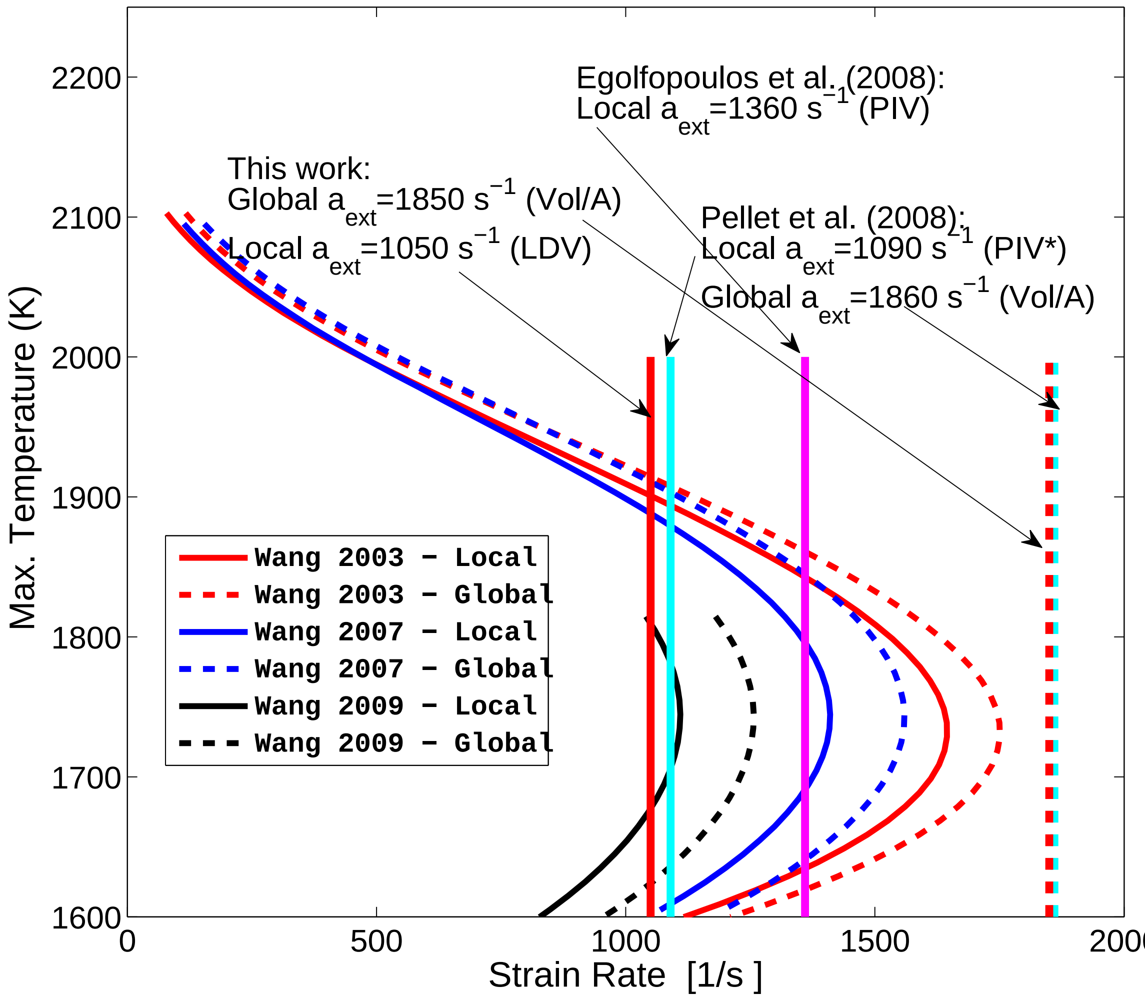
Some Definitions of Nonpremixed Flame Characteristics

- Global Strain Rate $a_{global} = 4\ v_{air}/L$ (Seshadri and Williams, 1978) where v_{air} from (i) Volume/Area, (ii) LDV/PIV, and (iii) computations.



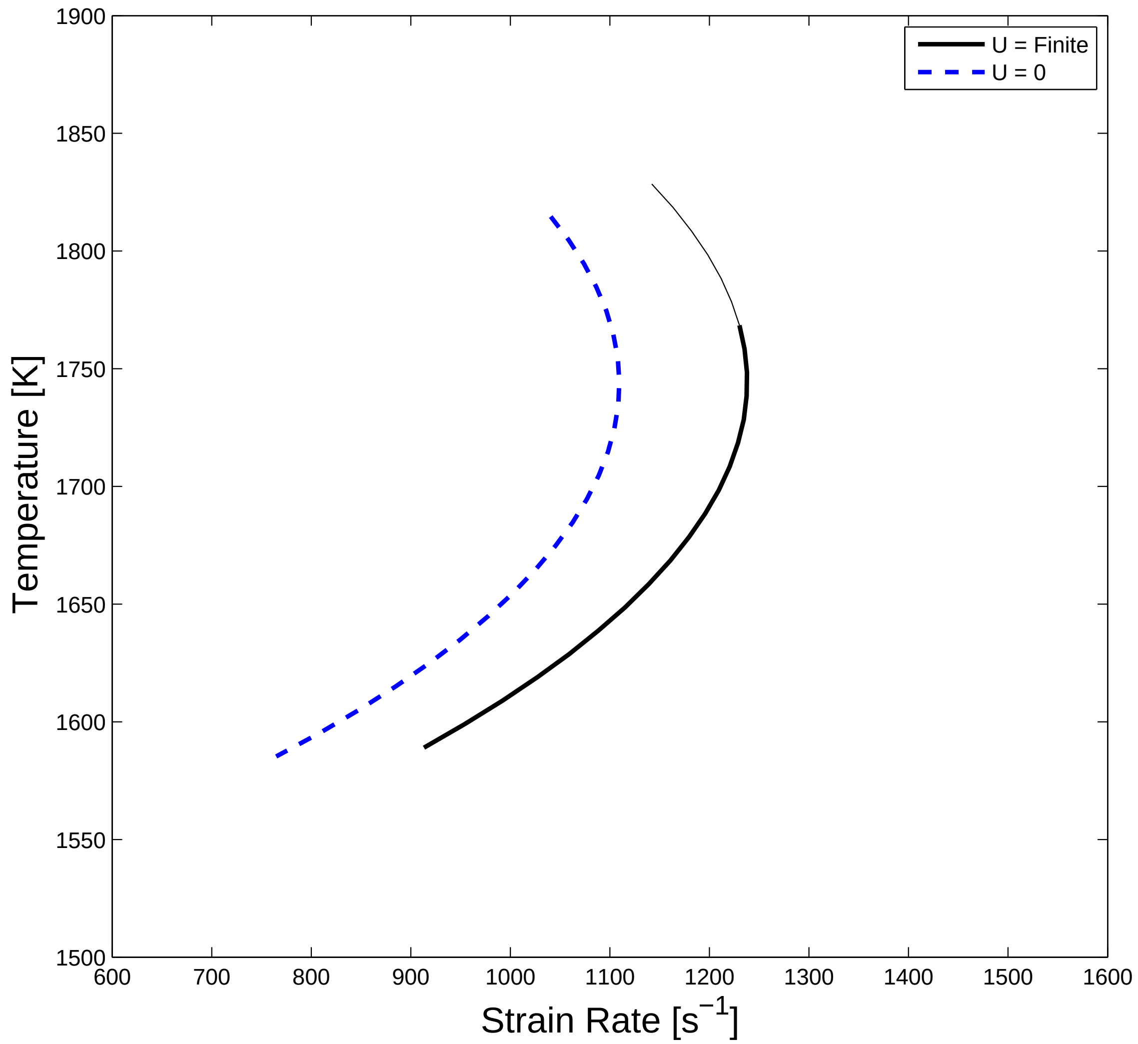
Extinction limit of ethylene-air Nonpremixed Flames

- ONE key uncertainty $\Rightarrow$ measurement of strain rate!
  - Experiments from USC, NASA Langley, and UVa.
  - Chemical kinetic models of Wang and co-workers.
  - Full Stefan-Maxwell Eq. to reduce uncertainty of diffusion



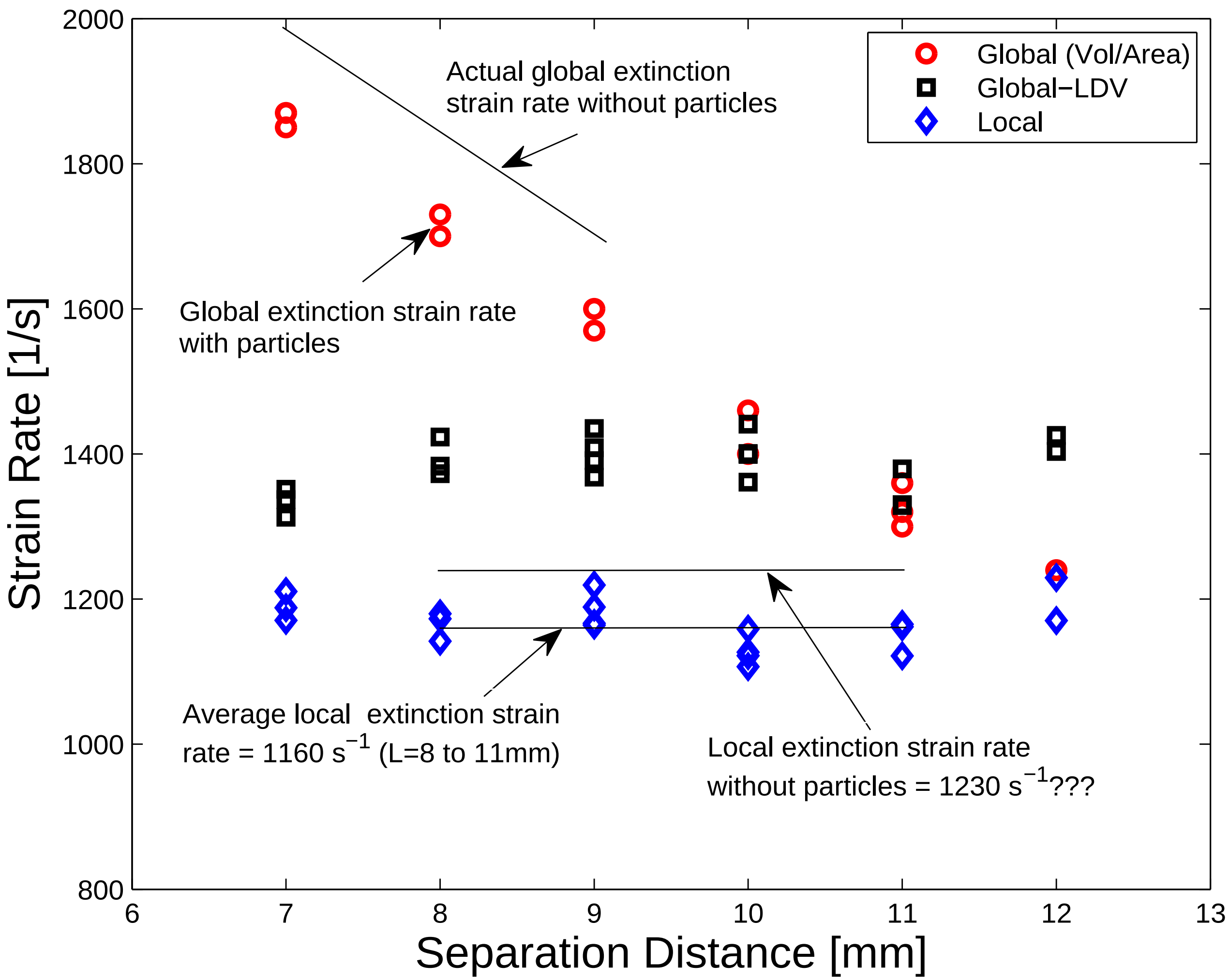
Influence of $U = 0$ vs. $U = Finite$ on Local Strain Rate

- $dv_z/dz + 2\rho U(z) = 0$ (Kee et al. 1988, Smooke et al., 1990)



Summary of Experimental Data and Uncertainties

- Particle seeding in LDV/PIV $\Rightarrow$ lower local strain rate?



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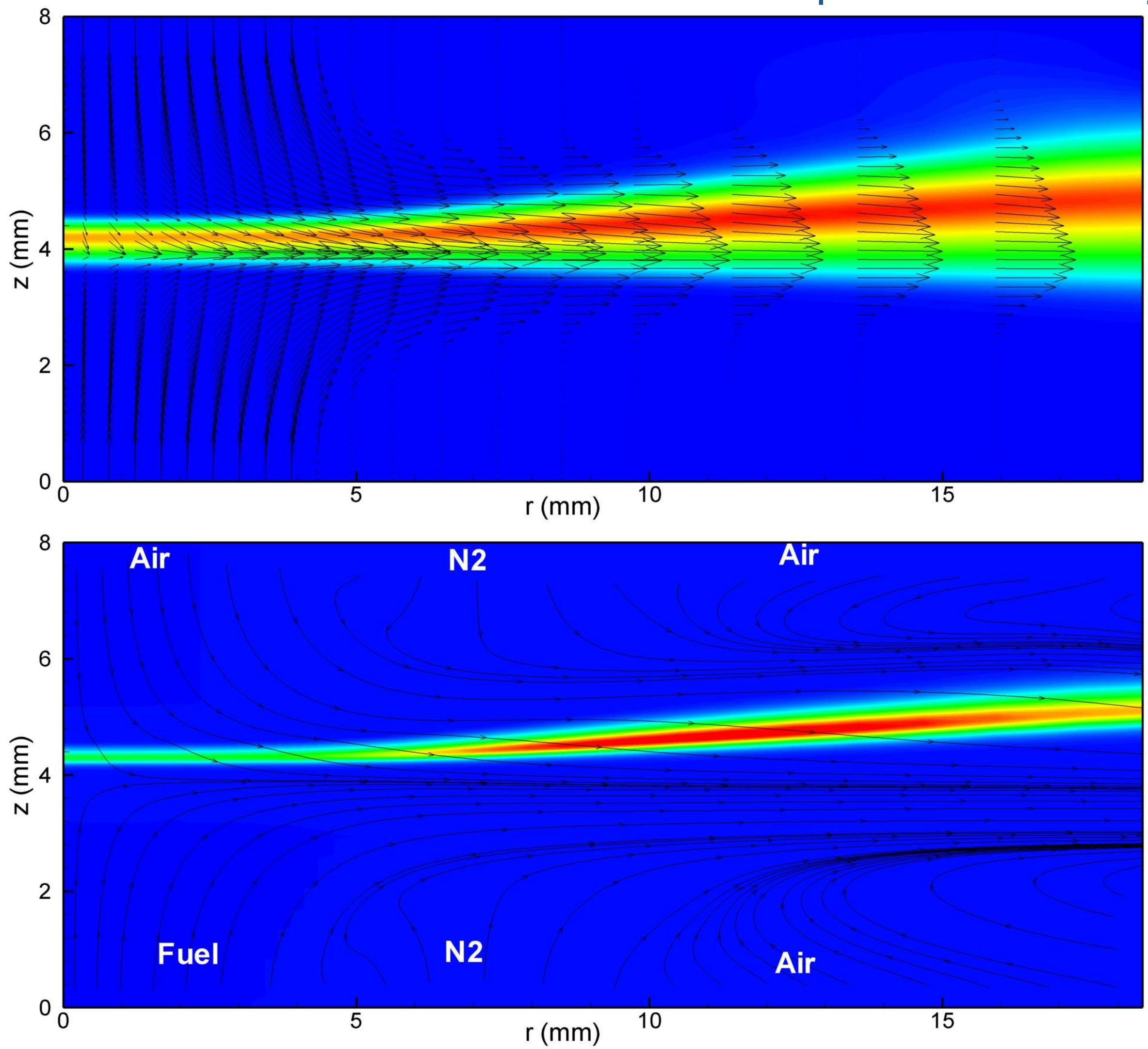
2D Axisymmetric Computations

- Amantini et al. (2007) considered a methane-air case
- Vish Katta's UNICORN code with USC Mech II Optimized for ethylene-air



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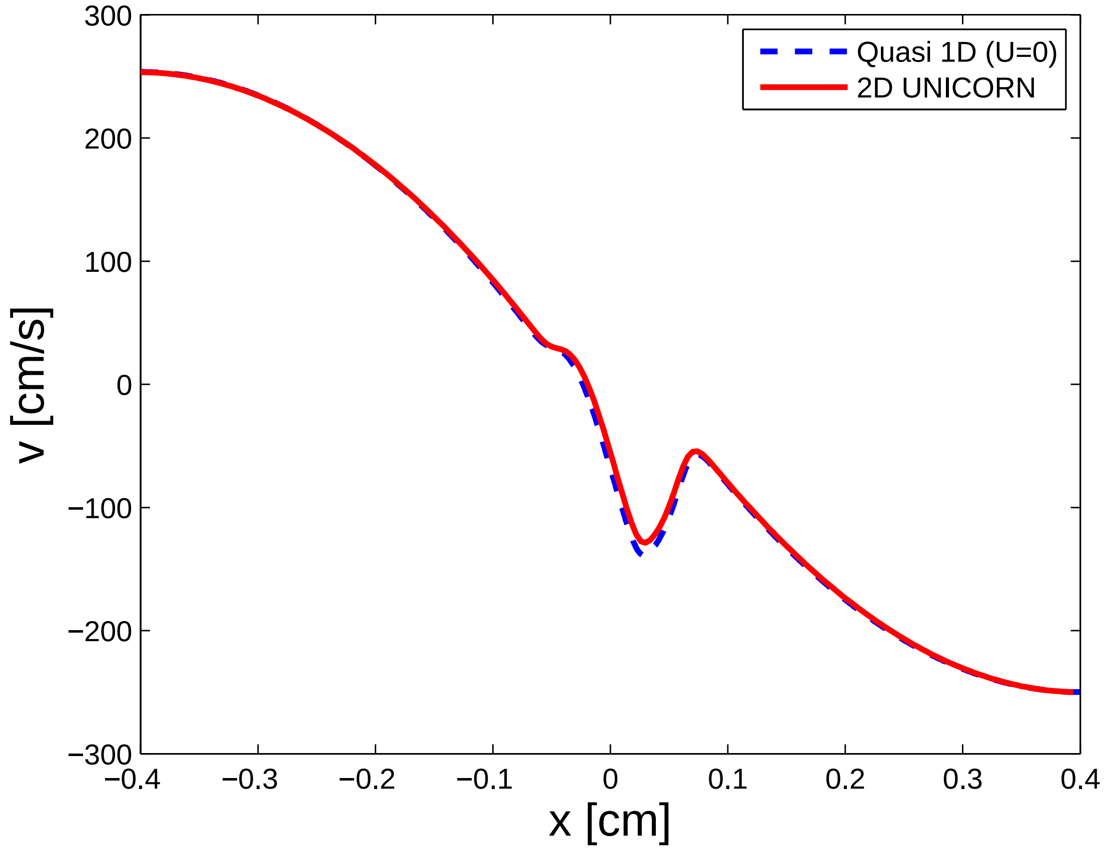

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Principal Component Analysis with Sensitivity (PCAS)

- Starting point of PCAS is the construction of response function (Vajda, Valko, and Turanyi (1985)):

$$Q(\mathbf{P}) = \sum_{j=1}^{q} \sum_{i=1}^{m} \left[\frac{f_i(x_j, \mathbf{P}) - f_i(x_j, \mathbf{P^0})}{f_i(x_j, \mathbf{P^0})} \right]^2$$

where $\mathbf{P}$, $\mathbf{P^0}$ are unperturbed and perturbed parameters ($k = 1, ..., p$); f_i a set of target functions ($i = 1, ..., m$); x_j collection of analysis points ($j = 1, ..., q$).

- Around $\mathbf{P^0}$, the response function can be approximated as:

$$Q(\mathbf{P}) \approx q(\mathbf{P}) = (\Delta\mathbf{P})^T \, \mathbf{S}^T\mathbf{S}(\Delta\mathbf{P}) = (\Delta\mathbf{P})^T \, \mathbf{U}^T \Lambda \mathbf{U}(\Delta\mathbf{P}) = \sum_{k=1}^{p} \lambda_k (\Delta\Psi_k)^2$$

where $\Delta\mathbf{P} = \mathbf{P} - \mathbf{P^0}$; $\mathbf{S}$ collection of sensitivity matricies; λ_k eigenvalues; $\mathbf{U}$ normalized eigenvectors; $\boldsymbol{\Delta\Psi} = \mathbf{U}^T\mathbf{P}$ principal components.

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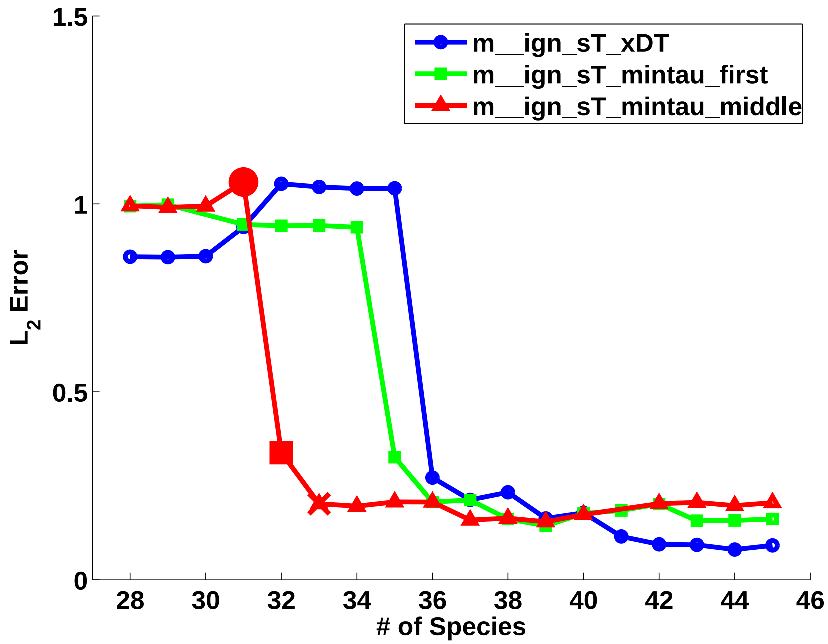
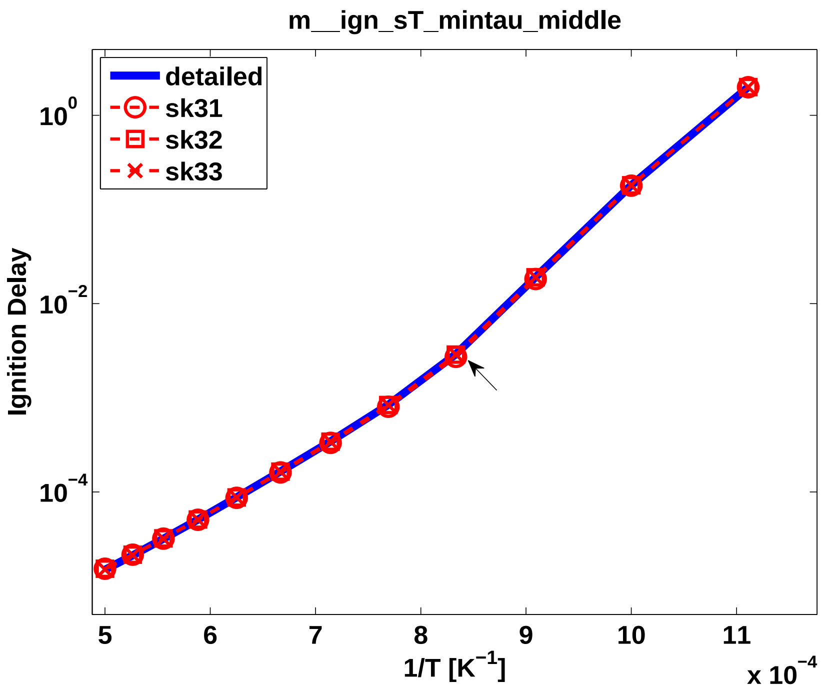
Application of PCAS to Ignition Delay

- Several key issues!!!
- Ethylene-air, p=1.0atm, ϕ=1.0 with Wang 2003 detailed model (71 species in 467 reactions)





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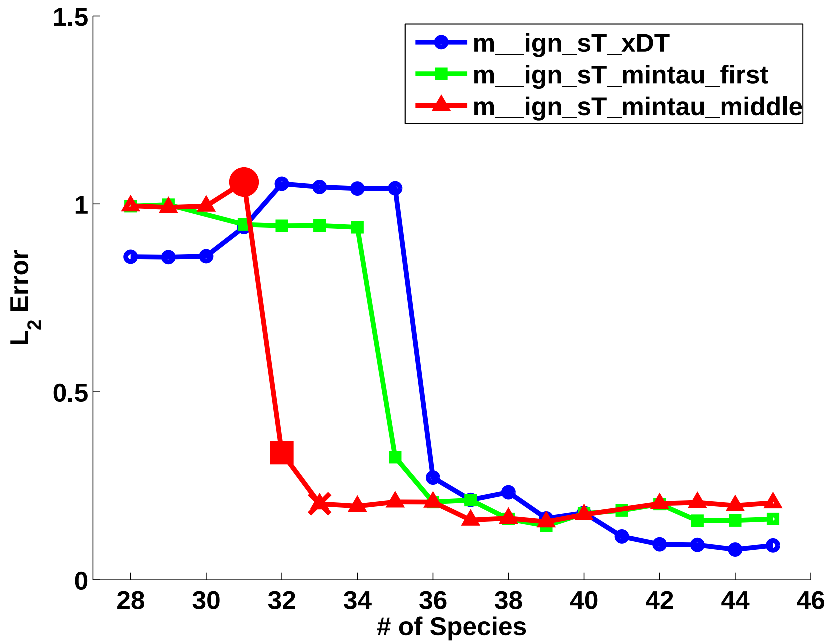
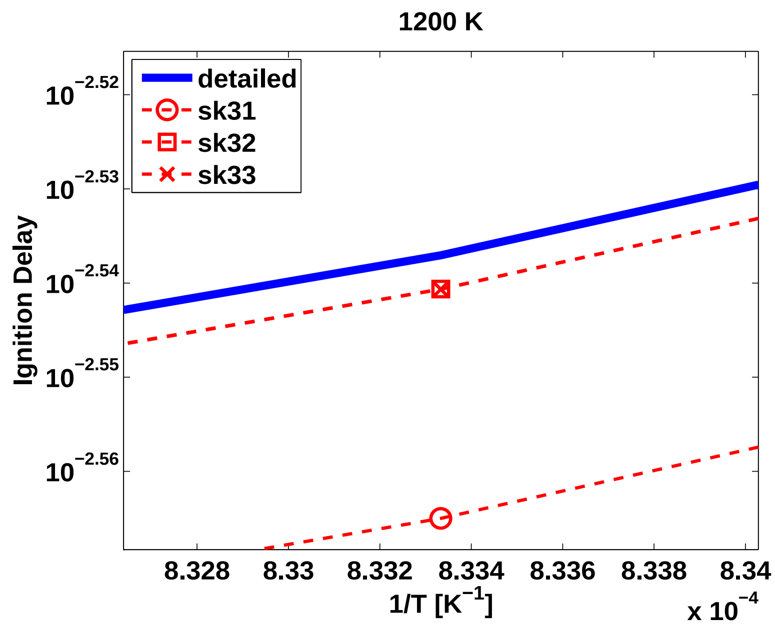
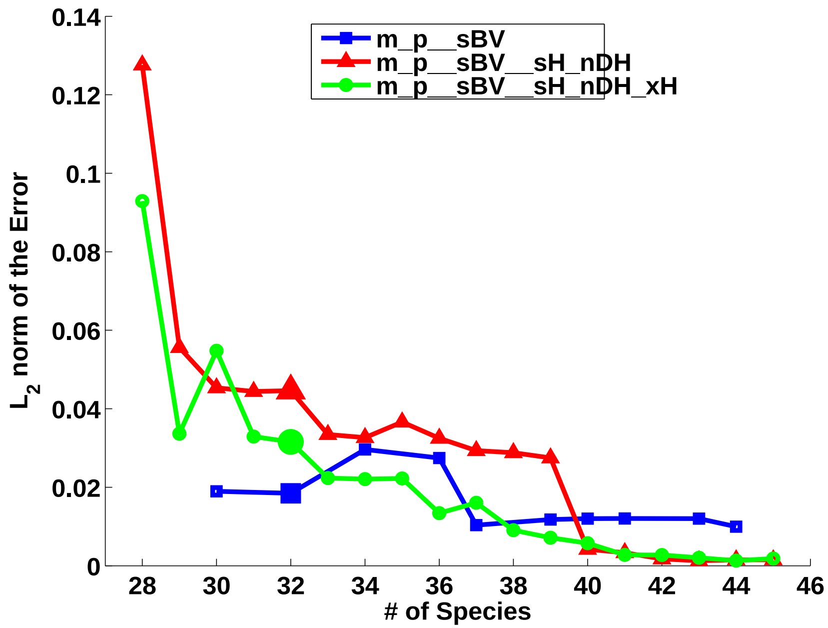
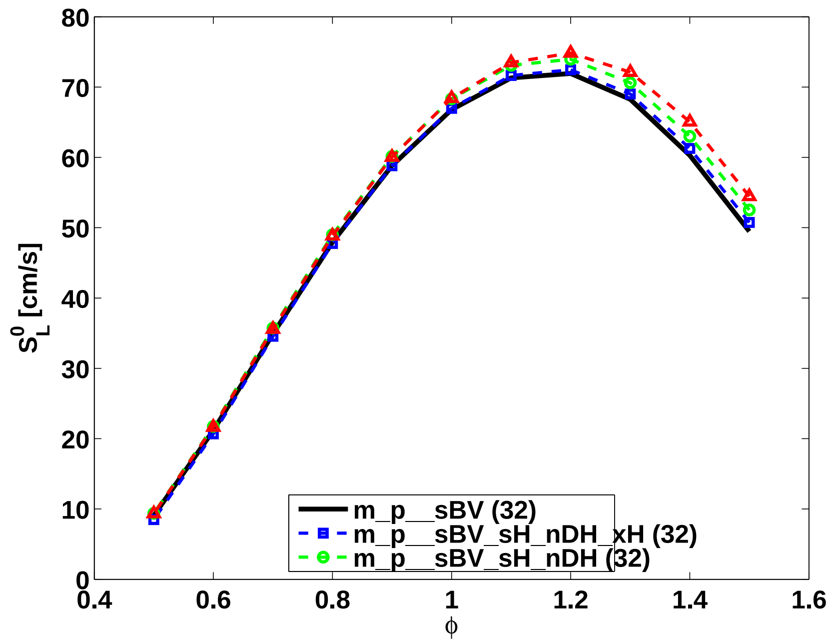




Application of PCAS to Flame Propagation

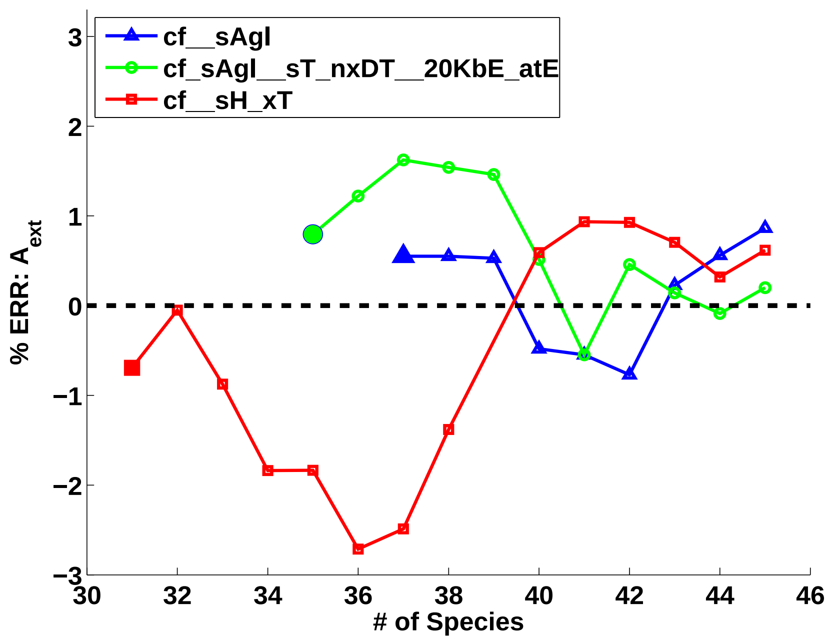
- Ethylene-air, p=1.0atm, T_0=300 K with Wang 2003 detailed model (71 species in 467 reactions)

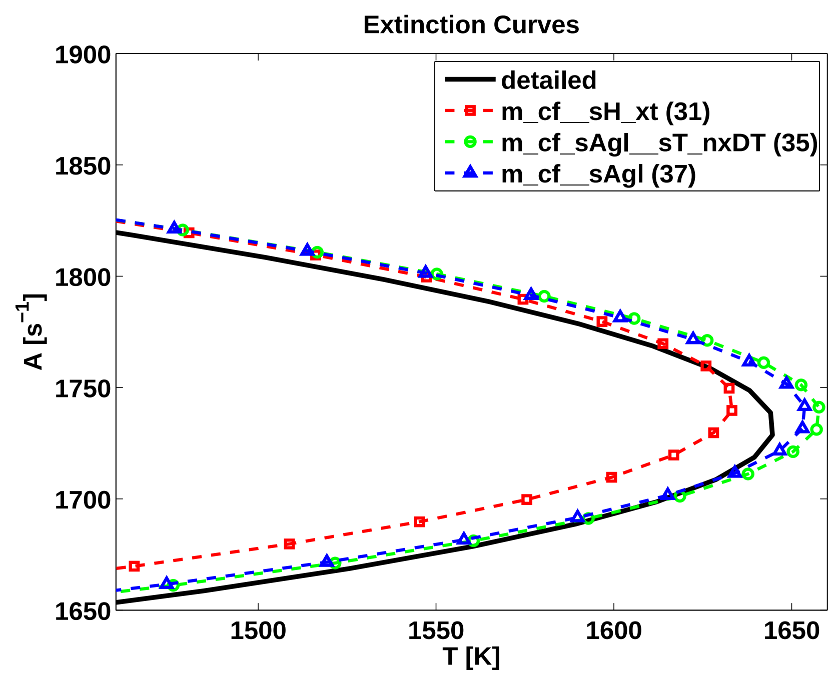




Application of PCAS to Flame Extinction

- Ethylene-air, p=1.0atm, T_0=300 K





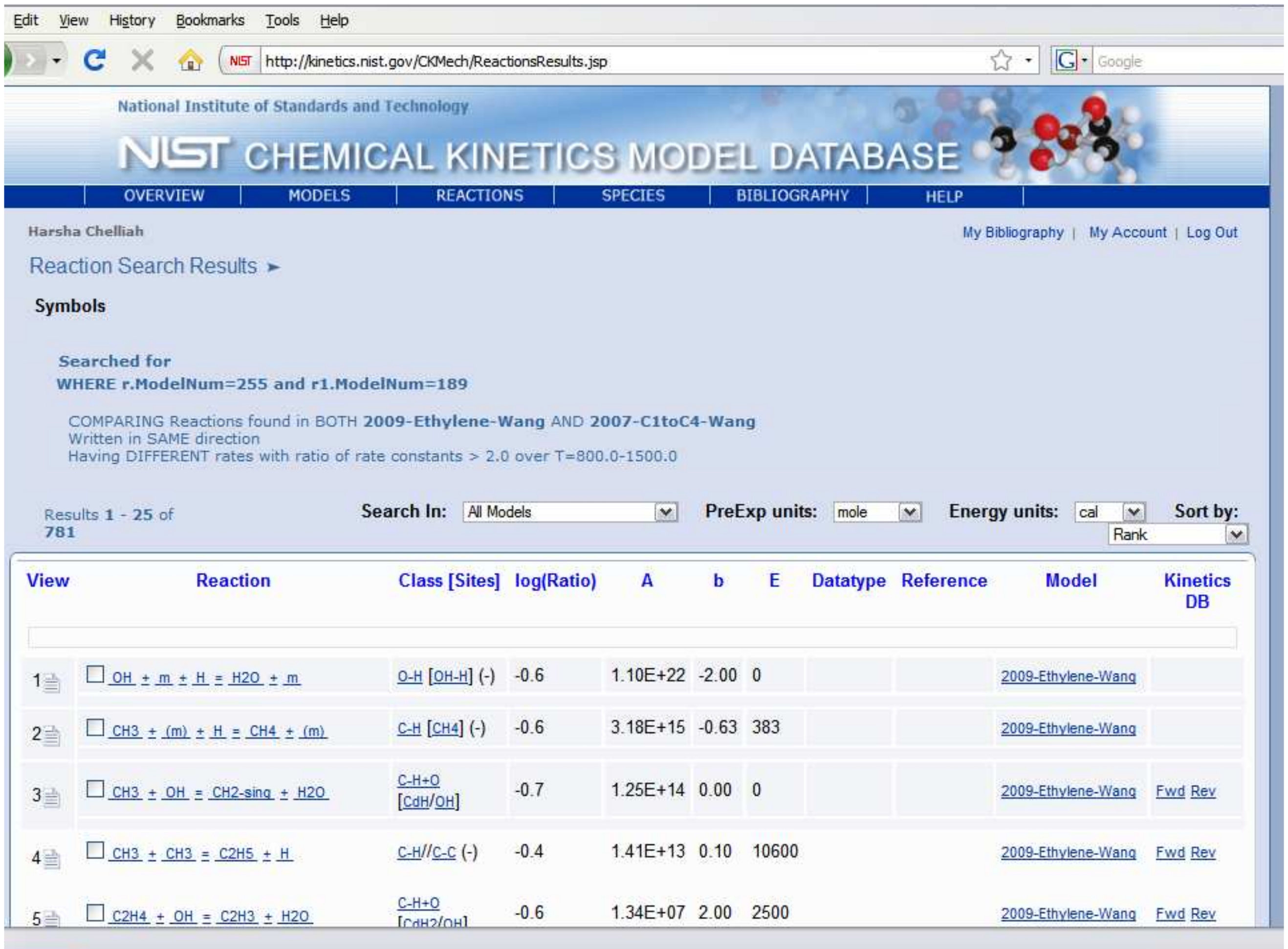
QSSA Reduction Approach

- QSSA Reduction Approach —- Zambon and Chelliah, *Combustion and Flame* (2007) — 15-step and 18-step reduced reaction models for ethylene-air based on a 31 species and 128 reaction skeletal model from Wang 2003.

- In the process of updating based on USC Mech II Optimized.

NIST Chemical Kinetics Database Program

- Extremely useful tool to analyze differences between chemical kinetic models (Don Burgess)



Concluding Remarks

- In quasi 1D extinction limit computations, $U = 0$ and $U = finite$ (from actual experiments) differ by nearly 10%!!!
- In extinction experiments with convergent nozzles, $L/D = 1$ case shows a non top-hat velocity profile $\Rightarrow$ main contributor to the differences between the measured local strain rate and the global strain rate
- Random errors (1160 ± 20) are too large to extract any systematic uncertainty associated with L/D variation
- detailed reaction models continue to evolve and may converge through collaborative based efforts like PrIME, this Fuels Group, ...

$\Rightarrow$ need to create accurate and independent experimental data with well-defined uncertainties

- automated reduction procedures are needed to take advantage of the evolving detailed reaction models (PCAS/QSSA, ...)

Acknowledgements

- Hai Wang for sharing kinetic models
- Wing Tsang, Jeff Manion, and Don Burgess at NIST
- OSD T&E and S&T, NASA Hypersonics NRA Program, and AFOSR/NASA National Center for Hypersonic Combined-Cycle Propulsion

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